ATOMISTIC MODELLING OF CROSS-SLIP AND ITS CONTRIBUTION TO THE UNDERSTANDING OF TEXTURE AND FATIGUE IN FCC MATERIALS

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Recent atomistic simulations of cross-slip of non-jogged screw dislocations in copper without stress assistance has produced activation energies of the order of 3eV, i.e. activation energies of a magnitude which would be prohibitively high for cross-slip at room temperature. However, subsequent atomistic simulations of the annihilation by cross-slip of non-jogged screw-dislocation dipoles in copper has shown that the attraction between the two dislocations in sufficiently narrow dipoles reduces the activation energy to a level which would allow cross slip at room temperature.

Jogs reduce the activation energy for cross-slip dramatically. Atomistic simulations of cross-slip of jogged screw dislocations in copper without stress assistance led to activation energies of ~0.9eV, which is comparable with the experimentally determined activation energy of 1.15eV. However, the activation volume for cross-slip derived by atomistic modelling $10b^3$, b being the Burgers vector – for non-jogged and jogged screw dislocations – is far smaller than that derived experimentally, $\sim 250b^3$.

In the present work we apply the above results derived by atomistic simulations in modelling of cross-slip on texture and fatigue in fcc materials. For the rolling-texture transition in fcc materials we find quantitative agreement between the experimental activation energy for the texture transition and the atomistically derived activation energy for cross-slip of jogged screw dislocations. For fatigue the atomistic results quantify several analytical models of nanostructural aspects of fatigue crack initiation in surface bulges and slip lines at persistent slip bands (PSBs). These models are all compatible with a recent nanotheory, which combines them to make definite quantitative predictions of the dislocation nanostructures induced by cyclic plasticity and of the nanoscale surface damage generated by heterogeneous PSB plasticity.